# Role of a Phase Factor in the Boundary Condition of a One-Dimensional Junction

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**Abstract.** One-dimensional quantum systems can be experimentally studied in recent nano-technology like the carbon nanotube and the nanowire. We have considered the mathematical model of the one-dimensional Schrödinger particle with a junction and have analyzed the phase factor in the boundary condition of the junction. We have shown that the phase factor in the tunneling case appears in the situation of the non-adiabatic transition with the three energy levels in the exact WKB analysis.

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## 1. Introduction

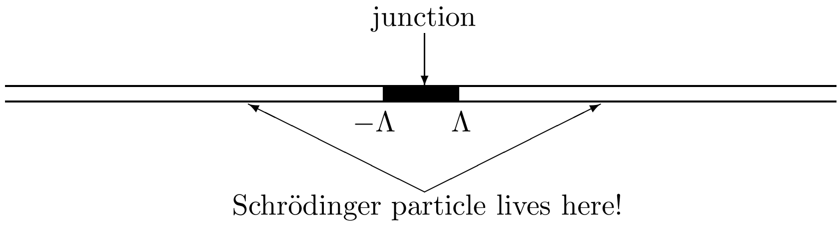
Quantum phases take the crucial role of the quantum interference and coherence. It is well known that the global phase factor for the quantum state is undetectable. On the other hand, since the relative phase is detectable by interference patterns such as the Young double-slit experiment for the electron [1] and the molecule [2], this quantity is meaningful. By the experimental demonstration of the delayed choice experiment or the quantum eraser [3], we know that this quantity depends on the operational set-up. Aharonov and Bohm predicted a phase of the electrically charged particle from an electromagnetic potential [4], which is known as the Aharonov-Bohm phase. Furthermore, Berry predicted a phase acquired over the course of a cycle with adiabatic processes resulting from the geometrical properties of the parameter space of the Hamiltonian [5], which is known as the Berry phase or the geometric phase. The Aharonov-Bohm phase [6, 7, 8] and the Berry phase [9, 10, 11] are experimentally realized. They are given by the Hamiltonian decided from the operational set-up. However, there also exists a phase factor in the boundary condition, which is not decided by the Hamiltonian but is decided by the situation of a quantum particle. In this paper we address the latter quantum phase under a one-dimensional system like the following physical set-up.

Recent development on experimental techniques has provided a way to study the one-dimensional quantum physics, for instance, see Ref. [12]. In this paper, we focus on the one-dimensional electron transport system. The electron on the single-wall carbon nanotube [13] and the nanowire made of semiconductor materials such as InP [14], InAs/InP [15], GaAs/GaP [14], and Si/SiGe [16] can be described as the one-dimensional quantum system. This can be controlled by the application of the technique on a single-electron transistor, which is a device in which electrons tunnel one at a time through a small island connected to two leads via a tunnel junction, in the single-wall carbon nanotube [17] and the InP nanowire [18]. Furthermore, two carbon nanotubes electrically can be connected via a junction such as a gold particle [19]. See more examples on the connected carbon nanotubes in Ref. [20]. We will consider a mathematical model of the one-dimensional quantum system with a junction throughout this paper.

As is well known, a physical observable is described by a self-adjoint operator [21]. Thus, the set $D(H)$ of all wave functions of a Hamiltonian $H$ should be determined so that $H$ becomes a self-adjoint operator. Usually, we begin with considering the action of an energy operator $H_0$ for the Hamiltonian $H$ on a domain $D(H_0)$ in which the energy operator $H_0$ is not self-adjoint since it is smaller than $D(H)$. Thus, we seek the Hamiltonian $H$ as an extension of $H_0$. This extension is called a *self-adjoint extension* [22]. As the boundary condition for a physical set-up is fixed, a self-adjoint extension is determined so that the extension corresponds to the boundary condition.

It is already known that a phase factor appears in a boundary condition for a self-adjoint extension of a momentum operator on a non-Euclidean space [22, 23]. In the

case of Hamiltonians, however, a phase factor does not always appear in the boundary condition, for instances, Example 2 in Ref. [22, §X.1], Theorem 3.1.1 in Ref. [24], and Eq. (1.1) in Ref. [25]. Thus, in this paper we make a realization of the above physical set-up to obtain a mathematical model to consider a Schrödinger particle in a line with a junction. In our mathematical idealization, the junction is represented by the closed interval $[-\Lambda, \Lambda]$ and the Schrödinger particle moves in $(-\infty, -\Lambda) \cup (\Lambda, \infty)$:




For example, we can take a non-relativistic electron as the Schrödinger particle ‡, and then, the junction is made from an insulator. We investigate the phase factor determined by the boundary conditions at the two edges ($x = -\Lambda$ and $x = \Lambda$) of the junction when the Schrödinger particle tunnels through the junction. In the near future we will consider controlling the phase factor determined by the boundary conditions using the Aharonov-Bohm phase obtained by a magnetic field through the junction only.

Our results characterize the boundary conditions for the point interaction given in Refs. [24] and [26] based on whether the Schrödinger particle tunnels through the junction or not. More precisely, the boundary condition in the case where the Schrödinger particle does not tunnel through the junction (as in Theorem 1) corresponds to that for the point interaction given in Ref. [24] (see Remark 1). On the other hand, the boundary condition in the case where the Schrödinger particle does tunnel through the junction (as in Theorems 2 and 3) corresponds to that for the point interaction given in Ref. [26] (see Remark 2). Namely, our results tell us that the generalized boundary condition given in the unfortunately unpublished paper [26] is important in the light of the Schrödinger particle tunneling the junction.

Our paper is constructed as follows. In Sec. 2 we recall some well-known facts and formulate our problem. In Sec. 3 we investigate the boundary conditions of wave functions, dividing them into two cases. In the first case we handle the Schrödinger particle not tunneling through the junction. In this case we can completely classify the type of boundary conditions of which type corresponds to that of in Ref. [24]. In other case we consider the Schrödinger particle tunneling through the junction. We give another type of boundary condition which corresponds to that for the point interaction given in Ref. [26]. Furthermore, this phase corresponds to one obtained by the exact WKB analysis in the model of the three-levels non-adiabatic transition inside the junction. Section 4 is devoted to the summary and the discussions.

‡ In the case of carbon nanotubes, the non-relativistic electron can be taken as the excitation of the Tomonaga-Luttinger liquid [20].

## 2. Preparations and Our Model

### *2.1. Mathematical Notations*

In this section, we prepare some mathematical terms and notions. For every operator $A$ acting in a Hilbert space, $D(A)$ expresses the set of all vectors on which the operator $A$ can act. For instance, $D(A)$ is the set of all wave functions as $A$ is an energy operator. $D(A)$ is called the *domain* of the operator $A$. For operators $A$ and $B$ we say $A$ is equal to $B$, i.e., $A = B$ if and only if $D(A) = D(B)$ and $A\psi = B\psi$ for every $\psi \in D(A) = D(B)$, where $\psi \in D(A)$ means the vector $\psi$ belongs to the domain $D(A)$. When $D(A) \subset D(B)$ and $A\psi = B\psi$ for every $\psi \in D(A)$, we say that the operator $B$ is an *extension* of the operator $A$, and we express that by $A \subset B$. $D(A^*)$ expresses the set of all vectors $\varphi$ satisfying the following for an operator $A$: there is a vector $\phi_{_A}$ so that $\langle\varphi|A\psi\rangle = \langle\phi_{_A}|\psi\rangle$ for every $\psi \in D(A)$. Then, the *adjoint operator* $A^*$ of the operator $A$ is given by $A^*\varphi = \phi_{_A}$ for every $\varphi \in D(A^*)$. Note that the domain $D(A^*)$ has to be dense in the Hilbert space since the adjoint operator $A^*$ is determined uniquely. The operator $A$ is said to be *symmetric* as $A \subset A^*$, and moreover, the operator $A$ *self-adjoint* if and only if $A = A^*$. Thus, when an operator $B$ is called a *self-adjoint extension* of an operator $A$, the operator $B$ satisfies $B = B^*$ and $A \subset B$. $D(\overline{A})$ expresses the set of all vectors $\psi$ satisfying the following conditions for an operator $A$: there is a sequence $\{\psi_n\}_n$ of vectors $\psi_n \in D(A)$ so that sequences $\{\psi_n\}_n$ and $\{A\psi_n\}_n$ converge, and $\psi = \lim_{n\to\infty}\psi_n$. Then, the *closure* $\overline{A}$ of the operator $A$ is defined by $\overline{A}\psi := \lim_{n\to\infty} A\psi_n$. We say that the operator $A$ is *closed* if $A = \overline{A}$. It is well known that a self-adjoint operator is closed.

Following Ref. [22, Example 2 in §X.1], we recapitulate some facts on self-adjoint extension here. For the subset $\Omega$ of the line $\mathbb{R} := (-\infty, \infty)$ $C_0^\infty(\Omega)$ expresses the set of all infinitely differentiable functions on $\Omega$ with their individual compact supports in $\Omega$. Here the support of a function $\psi$ on $\Omega$ is the closure $\overline{\{x \in \Omega \,|\, \psi(x) \neq 0\}}$ of the set $\{x \in \Omega \,|\, \psi(x) \neq 0\}$. $AC^2(\Omega)$ expresses the set of all absolutely continuous functions $\psi$ on $\Omega$ so that $\psi'$ is also absolutely continuous and $\psi''$ is square integrable on $\Omega$. It should be noted that the Lebesgue theorem states that absolutely continuous function $\psi$ has its differentiable $\psi'$ almost everywhere.

The regions $(-\infty, -\Lambda)$ and $(\Lambda, \infty)$ is denoted as $\Omega_{\rm L}$ and $\Omega_{\rm R}$ for an arbitrarily fixed constant $\Lambda > 0$, respectively. We define energy operators $H_{\rm L00}$ and $H_{\rm R00}$ by $H_{\rm L00} := -d^2/dx^2$ with $D(H_{\rm L00}) := C_0^\infty(\Omega_{\rm L})$ and $H_{\rm R00} := -d^2/dx^2$ with $D(H_{\rm R00}) := C_0^\infty(\Omega_{\rm R})$ respectively. Set $H_{\rm L0}$ and $H_{\rm R0}$ as $H_{\rm L0} := \overline{H_{\rm L00}}$ and $H_{\rm R0} := \overline{H_{\rm R00}}$. Then, similarly to proof of Ref. [22, Example 2 in §X.1], all self-adjoint extensions of $H_{\rm L0}$ and $H_{\rm R0}$ are represented with real parameters $\alpha_{_{\rm L}}$ and $\alpha_{_{\rm R}}$ in the following: For every $\alpha_{_{\rm L}} \in \mathbb{R}$, we have the self-adjoint extension

$$H_{\alpha_{_{\rm L}}} = -\frac{d^2}{dx^2} \;\text{ with }\; D(H_{\alpha_{_{\rm L}}}) = \left\{\psi \in AC^2(\overline{\Omega_{\rm L}}) \,|\, \psi'(-\Lambda) = \alpha_{_{\rm L}}\psi(-\Lambda)\right\}, \quad (1)$$

and for $\alpha_{_{\rm L}} = \infty$, we have the self-adjoint extension

$$H_\infty = -\frac{d^2}{dx^2} \;\text{ with }\; D(H_\infty) = \left\{\psi \in AC^2(\overline{\Omega_{\rm L}}) \,|\, \psi'(-\Lambda) = 0\right\}. \quad (2)$$

Similarly, for every $\alpha_{\mathrm{R}} \in \mathbb{R}$, we have the self-adjoint extension

$$H_{\alpha_{\mathrm{R}}} = -\frac{d^2}{dx^2} \ \text{with} \ D(H_{\alpha_{\mathrm{R}}}) = \left\{ \psi \in AC^2(\overline{\Omega_{\mathrm{R}}}) \,|\, \psi'(\Lambda) = \alpha_{\mathrm{R}} \psi(\Lambda) \right\}, \tag{3}$$

and for $\alpha_{\mathrm{R}} = \infty$, we have the self-adjoint extension

$$H_{\infty} = -\frac{d^2}{dx^2} \ \text{with} \ D(H_{\infty}) = \left\{ \psi \in AC^2(\overline{\Omega_{\mathrm{R}}}) \,|\, \psi'(\Lambda) = 0 \right\}. \tag{4}$$

Here $\overline{\Omega}$ denotes the closure of a set $\Omega \subset \mathbb{R}$.

### *2.2. Mathematical Setups for Our Model*

In this paper, the closed interval $[-\Lambda, \Lambda]$ represents a junction on the line for an arbitrarily fixed constant $\Lambda > 0$. We define a one-dimensional, the non-Euclidean space $\Omega_\Lambda$ by eliminating the junction from the line $(-\infty, \infty)$, i.e., $\Omega_\Lambda := (-\infty, -\Lambda) \cup (\Lambda, \infty)$. We assume that a free Schrödinger particle such as a non-relativistic electron lives in $\Omega_\Lambda$. To consider self-adjoint extensions $H$ as Hamiltonians of the particle, we begin with giving the action $H_{00}$ of the energy operator with a small domain $D(H_{00})$ in which $H_{00}$ is not self-adjoint yet since it is smaller than $D(H)$. In the next section we will show how a self-adjoint extension is determined so that the extension corresponds to the boundary condition of each physical set-up.

We consider the Hilbert space $L^2(\Omega_\Lambda)$ defined as the set of all square integrable functions on $\Omega_\Lambda$. This represents the state space to which wave functions of our Schrödinger particle belong. The energy operator $H_{00}$ is defined by

$$H_{00} := -\frac{d^2}{dx^2} \ \text{with} \ D(H_{00}) := C_0^\infty(\Omega_\Lambda). \tag{5}$$

Then, although the operator $H_{00}$ is neither closed nor self-adjoint, $H_{00}$ is symmetric. We denote the closure of $H_{00}$ by $H_0$, i.e., $H_0 := \overline{H_{00}}$. Then, by the well-known theorem that $H_0^* = H_{00}^*$, and moreover, $H_0 \subset H_0^*$. So, $H_0$ is symmetric, though $H_0^*$ is *not* symmetric. Thus, $H_0^*$ has some purely imaginary eigenvalues. Then, as in Definition in Ref. [22, §X.1], we define vector spaces $\mathcal{H}_+(H_0)$ and $\mathcal{H}_-(H_0)$ by $\mathcal{H}_+(H_0) := \{\psi \in D(H_0^*) \,|\, H_0^*\psi = i\psi\}$ and $\mathcal{H}_-(H_0) := \{\psi \in D(H_0^*) \,|\, H_0^*\psi = -i\psi\}$ respectively. We call $\mathcal{H}_+(H_0)$ and $\mathcal{H}_-(H_0)$ the *deficiency subspaces.*

We can respectively prove the first part of the following proposition in the same way as the proof of Ref. [27, Theorem 8.25(b)] and the second part similarly to the proof of Ref. [27, Theorem 8.22] (see also Ref. [28, Example 3 in §VIII.6]):

**Proposition 1.** *The operators $H_0$ and $H_0^*$ have the following actions with the domains respectively:*

$$H_0 = -\frac{d^2}{dx^2}$$
$$\textit{with} \ D(H_0) = \{\psi \in D(H_0^*) \,|\, \psi(-\Lambda) = \psi(\Lambda) = \psi'(-\Lambda) = \psi'(\Lambda) = 0\}, \tag{6}$$

*and*

$$H_0^* = -\frac{d^2}{dx^2} \ \textit{with} \ D(H_0^*) = \left\{ \psi \in L^2(\Omega_\Lambda) \,|\, \psi \in AC^2(\overline{\Omega_\Lambda}) \right\}. \tag{7}$$

Theorem X.2 of Ref. [22], together with its corollary and Proposition 1, says that for every self-adjoint extension $H_{U}$ of $H_0$ there is a unitary operator $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ so that $H_{U} = -d^2/dx^2$ with the domain:

$$D(H_{U}) = \{\psi_0 + \psi_+ + U\psi_+ \,|\, \psi_0 \in D(H_0), \psi_+ \in \mathcal{H}_+(H_0)\}\,. \tag{8}$$

Conversely, for every unitary operator $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ the operator $H_{U} = -d^2/dx^2$ with the domain given by Eq. (8) is a self-adjoint extension of $H_0$. That is, the self-adjoint extensions $H_{U}$ of $H_0$ are in one-to-one correspondence with the set of all unitary operators $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$.

Solving simple differential equations, we can obtain the eigenfunctions $R_\pm$ and $L_\pm$ of $H_0^*$:

$$R_+(x) := \begin{cases} 0 & \text{if } -\infty < x < \Lambda, \\ Ne^{(-1+i)x/\sqrt{2}} & \text{if } \Lambda < x < \infty, \end{cases} \tag{9}$$

$$R_-(x) := \begin{cases} 0 & \text{if } -\infty < x < \Lambda, \\ Ne^{(-1-i)x/\sqrt{2}} & \text{if } \Lambda < x < \infty, \end{cases} \tag{10}$$

and

$$L_+(x) := \begin{cases} Ne^{(1-i)x/\sqrt{2}} & \text{if} -\infty < x < \Lambda, \\ 0 & \text{if } \Lambda < x < \infty, \end{cases} \tag{11}$$

$$L_-(x) := \begin{cases} Ne^{(1+i)x/\sqrt{2}} & \text{if } -\infty < x < \Lambda, \\ 0 & \text{if } \Lambda < x < \infty, \end{cases} \tag{12}$$

with the normalization factor $N = \sqrt[4]{2}e^{\Lambda/\sqrt{2}}$ so that $H_0^* R_\pm = \pm i R_\pm$ and $H_0^* L_\pm = \pm i L_\pm$. Namely, $L_+, R_+ \in \mathcal{H}_+(H_0)$ and $L_-, R_- \in \mathcal{H}_-(H_0)$. The uniqueness of the differential equations tells us that

$$\mathcal{H}_+(H_0) = \{c_{\mathrm{L}} L_+ + c_{\mathrm{R}} R_+ \,|\, c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}\}\,, \tag{13}$$

$$\mathcal{H}_-(H_0) = \{c_{\mathrm{L}} L_- + c_{\mathrm{R}} R_- \,|\, c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}\}\,, \tag{14}$$

and thus, the dimensions of $\mathcal{H}_+(H_0)$ and $\mathcal{H}_-(H_0)$ are given as $\dim \mathcal{H}_+(H_0) = 2 = \dim \mathcal{H}_-(H_0)$, respectively §. This says that the set of all unitary operators $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ makes $SU(2)$, and thus, that the unitary operator $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ is given either by

$$UL_+ = \gamma_{\mathrm{L}} L_- \quad \text{and} \quad UR_+ = \gamma_{\mathrm{L}} R_- \tag{15}$$

for some $\gamma_{\mathrm{L}}, \gamma_{\mathrm{R}} \in \mathbb{C}$ with $|\gamma_{\mathrm{L}}| = 1 = |\gamma_{\mathrm{R}}|$ or by

$$UL_+ = \gamma_{\rightarrow} R_- \quad \text{and} \quad UR_+ = \gamma_{\leftarrow} L_- \tag{16}$$

for some $\gamma_{\rightarrow}, \gamma_{\leftarrow} \in \mathbb{C}$ with $|\gamma_{\rightarrow}| = 1 = |\gamma_{\leftarrow}|$. Let us denote the vector $(\gamma_{\mathrm{L}}, \gamma_{\mathrm{R}})$ or $(\gamma_{\rightarrow}, \gamma_{\leftarrow})$ by $\gamma$. Then, using the one-to-one correspondence $U \longleftrightarrow \gamma$ given by Eqs. (15) and (16),

§ The densely defined symmetric operators can be classified by the *deficiency theorem* ( see Refs. [36] and [37, Appendix B] for physicists) using the dimensions of the deficiency subspaces. In the case of $\dim \mathcal{H}_+(H_0) = \dim \mathcal{H}_-(H_0)$, $H_0$ has a self-adjoint extension due to the deficiency theorem.

we can represent $H_U$ by $H_\gamma$. Thus, seeking a self-adjoint extension of $H_0$ is equivalent to finding a $H_\gamma$ with $H_0 \subset H_\gamma = H_\gamma^* \subset H_0^*$ for a unitary operator $U$, that is, a vector $\gamma = (\gamma_{\mathrm{L}}, \gamma_{\mathrm{R}})$ or $\gamma = (\gamma_\to, \gamma_\leftarrow)$.

To find a boundary condition that a self-adjoint extension $H_\gamma$ of $H_0$ satisfies, we use the following tool:

$$W(\varphi, \phi) := W_{-\Lambda}(\varphi^*, \phi) - W_\Lambda(\varphi^*, \phi) \tag{17}$$

for all vectors $\varphi, \phi \in D(H_0^*)$, where $W_x(f,g)$ is the Wronskian: $W_x(f,g) := f'(x)g(x) - f(x)g'(x)$.

## 3. Phase Factor in Boundary Conditions

In this section we investigate boundary conditions when the Schrödinger particle both does and does not tunnel through the junction.

### *3.1. Non-Tunneling Schrödinger Particle*

Following Eqs.(8) and (15), wave functions $\psi$ of a self-adjoint extension of $H_0$ is given as $\psi = \psi_0 + (c_{\mathrm{L}} L_- + c_{\mathrm{R}} R_-) + (c_{\mathrm{L}} U L_- + c_{\mathrm{R}} U R_-)$, where $\psi_0 \in D(H_0)$, $c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}$. Thus, in the case where $\psi$ does not tunnel through the junction, the unitary operator $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ should be given by $UL_+ = \gamma_{\mathrm{L}} L_-$ and $UR_+ = \gamma_{\mathrm{R}} R_-$ for some $\gamma_{\mathrm{L}}, \gamma_{\mathrm{R}} \in \mathbb{C}$ with $|\gamma_{\mathrm{L}}| = 1 = |\gamma_{\mathrm{R}}|$. Namely, wave functions $\psi$ have the form of

$$\psi = \psi_0 + c_{\mathrm{L}}(L_+ + \gamma_{\mathrm{L}} L_-) + c_{\mathrm{R}}(R_+ + \gamma_{\mathrm{R}} R_-), \tag{18}$$

and moreover, the boundary conditions of $\psi(-\Lambda)$ and $\psi'(-\Lambda)$ are independent of those of $\psi(\Lambda)$ and $\psi'(\Lambda)$. Because any wave function $\psi_{\mathrm{L}}$ on the island $(-\infty, -\Lambda)$ and any wave function $\psi_{\mathrm{R}}$ on the island $(\Lambda, \infty)$ are isolated from each other. In this case, $\psi$ has to be mathematically equivalent to $\psi \cong \psi_{\mathrm{L}} \oplus \psi_{\mathrm{R}}$ with $\psi_{\mathrm{L}} = \psi_{\mathrm{L}0} + c_{\mathrm{L}}(L_+ + \gamma_{\mathrm{L}} L_-)$ and $\psi_{\mathrm{R}} = \psi_{\mathrm{R}0} + c_{\mathrm{R}}(R_+ + \gamma_{\mathrm{R}} R_-)$. Here we note that there are wave functions $\psi_{\mathrm{L}0} \in D(H_{\mathrm{L}0})$ and $\psi_{\mathrm{R}0} \in D(H_{\mathrm{R}0})$ so that $\psi_0 = \psi_{\mathrm{L}0} \oplus \psi_{\mathrm{R}0}$. Thus, any self-adjoint extension $H_\alpha$ without tunneling should be divided into the Schrödinger operators $H_{\alpha_{\mathrm{L}}}$ and $H_{\alpha_{\mathrm{R}}}$ as follows:

$$H_\alpha \cong H_{\alpha_{\mathrm{L}}} \oplus H_{\alpha_{\mathrm{R}}}, \tag{19}$$

using self-adjoint extensions shown in Eqs. (1), (2), (3), and (4), where $I$ denotes the identity operator.

The following theorem and proposition establish the above physical image. Namely, we can classify self-adjoint extensions of $H_0$ of which wave functions cannot tunnel through the junction in the following:

**Theorem 1.** *(i) Define the action of the Hamiltonian $H_\gamma$ by $H_\gamma := -d^2/dx^2$ with $\gamma := (\gamma_{\mathrm{L}}, \gamma_{\mathrm{R}})$, and give its domain $D(H_\gamma)$ by the set of all wave functions $\psi$ satisfying Eq. (18):*

$$D(H_\gamma) := \{\psi_0 + c_{\mathrm{L}}(L_+ + \gamma_{\mathrm{L}} L_-) + c_{\mathrm{R}}(R_+ + \gamma_{\mathrm{R}} R_-) \mid \psi_0 \in D(H_0),\, c_{\mathrm{L}},\, c_{\mathrm{R}} \in \mathbb{C}\}. \tag{20}$$

*If* $\gamma_{\rm L}$ *and* $\gamma_{\rm R}$ *are given by* $\gamma_{\rm L} := e^{i(\theta_{\rm L}+\sqrt{2}\Lambda)}$ *and* $\gamma_{\rm R} := e^{i(\theta_{\rm R}+\sqrt{2}\Lambda)}$ *for* $0 \le \theta_{\rm L}, \theta_{\rm R} < 2\pi$, *then* $H_\gamma$ *is a self-adjoint extension of* $H_0$.

*(ii) Define the action of the Hamiltonian* $H_\alpha$ *by* $H_\alpha := -d^2/dx^2$ *with* $\alpha := (\alpha_{\rm L}, \alpha_{\rm R})$, *where* $\alpha_{\rm L}, \alpha_{\rm R} \in \mathbb{R} \cup \{\infty\}$. *If the domain* $D(H_\alpha)$ *is given by one of (a)–(d):*

*(a) for* $\alpha \in \mathbb{R}\times\mathbb{R}$,

$$D(H_\alpha) := \{\psi \in D(H_0^*) \,|\, \psi'(-\Lambda) = \alpha_{\rm L}\psi(-\Lambda) \ \textit{and}\ \psi'(\Lambda) = \alpha_{\rm R}\psi(\Lambda)\}\,; \tag{21}$$

*(b) for* $\alpha \in \mathbb{R}\times\{\infty\}$,

$$D(H_\alpha) := \{\psi \in D(H_0^*) \,|\, \psi'(-\Lambda) = \alpha_{\rm L}\psi(-\Lambda) \ \textit{and}\ \psi'(\Lambda) = 0\}\,; \tag{22}$$

*(c) for* $\alpha \in \{\infty\}\times\mathbb{R}$,

$$D(H_\alpha) := \{\psi \in D(H_0^*) \,|\, \psi'(-\Lambda) = 0 \ \textit{and}\ \psi'(\Lambda) = \alpha_{\rm R}\psi(\Lambda)\}\,; \tag{23}$$

*(d) for* $\alpha = (\infty, \infty)$,

$$D(H_\alpha) := \{\psi \in D(H_0^*) \,|\, \psi'(-\Lambda) = 0 = \psi'(\Lambda)\}\,; \tag{24}$$

*then* $H_\alpha$ *is a self-adjoint extension of* $H_0$.

*(iii) Every self-adjoint extension* $H_\gamma$ *as in part (i) and every self-adjoint extension* $H_\alpha$ *as in part (ii) become equal to each other (i.e.,* $H_\alpha = H_\gamma$*) with the one-to-one correspondence,* $(\mathbb{C}\cup\{\infty\})\times(\mathbb{C}\cup\{\infty\}) \longrightarrow [0,2\pi)\times[0,2\pi)$ *:*

$$\alpha_{\rm L} = \frac{1+\cos\theta_{\rm L} - \sin\theta_{\rm L}}{\sqrt{2}(1+\cos\theta_{\rm L})} \quad \textit{and} \quad \alpha_{\rm R} = -\frac{1+\cos\theta_{\rm R} - \sin\theta_{\rm R}}{\sqrt{2}(1+\cos\theta_{\rm R})}, \tag{25}$$

*where* $\alpha_\sharp = \infty$ *if* $\theta_\sharp = \pi$, $\sharp = \mathrm{L}, \mathrm{R}$. *Therefore,* $H_\alpha$ *is equivalent to* $H_{\alpha_{\rm L}} \oplus H_{\alpha_{\rm R}}$, *i.e.,*

$$H_\alpha \cong H_{\alpha_{\rm L}} \oplus H_{\alpha_{\rm R}}. \tag{26}$$

Before proving Theorem 1, the following lemma which is easily proved in the same way as in Ref. [22, Example 2 in §X.1]:

**Lemma 1.** *Let* $\theta_{\rm L}, \theta_{\rm R} \in [0,\pi)\cup(\pi,2\pi)$ *and* $\alpha_{\rm L}, \alpha_{\rm R} \in \mathbb{R}$ *be arbitrarily given. Then, any subspace* $D(H_\gamma)$ *as in Theorem 1 (i) and any subspace* $D(H_\alpha)$ *as in Theorem 1 ((ii)a) are equal if and only if the following correspondence holds:*

$$\begin{cases} \sqrt{2}(1+\cos\theta_{\rm L})\alpha_{\rm L} = 1+\cos\theta_{\rm L} - \sin\theta_{\rm L}, \\ \sqrt{2}(1+\cos\theta_{\rm R})\alpha_{\rm R} = -\,(1+\cos\theta_{\rm R} - \sin\theta_{\rm R})\,, \end{cases} \tag{27}$$

*where*

$$\gamma_{\rm L} = e^{i(\theta_{\rm L}+\sqrt{2}\Lambda)} \ \textit{and}\ \gamma_{\rm R} = e^{i(\theta_{\rm R}+\sqrt{2}\Lambda)}. \tag{28}$$

*Proof.* Assume $D(H_\gamma) = D(H_\alpha)$. Take an arbitrary vector $\psi \in D(H_\gamma)$. It is equivalent to take the vector $\psi = \psi_0 + c_{\rm L}L_+ + c_{\rm R}R_+ + c_{\rm L}\gamma_{\rm L}L_- + c_{\rm R}\gamma_{\rm R}R_-$ for arbitrary $c_{\rm L}, c_{\rm R} \in \mathbb{C}$ and arbitrary $\psi_0 \in D(H_0)$. By the boundary condition as in Theorem 1 ((ii)a), we have

$$\begin{cases} \frac{1-i}{\sqrt{2}}c_{\rm L}L_+(-\Lambda) + \frac{1+i}{\sqrt{2}}c_{\rm L}\gamma_{\rm L}L_-(-\Lambda) = \alpha_{\rm L}c_{\rm L}L_+(-\Lambda) + \alpha_{\rm L}c_{\rm L}\gamma_{\rm L}L_-(-\Lambda), \\ \frac{-1+i}{\sqrt{2}}c_{\rm R}R_+(\Lambda) + \frac{-1-i}{\sqrt{2}}c_{\rm R}\gamma_{\rm R}R_-(\Lambda) = \alpha_{\rm R}c_{\rm R}R_+(\Lambda) + \alpha_{\rm R}c_{\rm R}\gamma_{\rm R}R_-(\Lambda). \end{cases} \tag{29}$$

It should be noted that

$$\begin{cases} L_+(-\Lambda) = R_+(\Lambda), \\ L_-(-\Lambda) = R_-(\Lambda) = R_+(\Lambda)^*, \end{cases} \tag{30}$$

and

$$R_+(\Lambda) = R_+(\Lambda)^* e^{i\sqrt{2}\Lambda}. \tag{31}$$

Using Eqs. (29) – (31), since $c_{\mathrm{L}}$ and $c_{\mathrm{R}}$ are arbitrary, we obtain

$$\begin{cases} \frac{1-i}{\sqrt{2}} + \frac{1+i}{\sqrt{2}} e^{i\theta_{\mathrm{L}}} = \alpha_{\mathrm{L}}(1 + e^{i\theta_{\mathrm{L}}}), \\ \frac{-1+i}{\sqrt{2}} + \frac{-1-i}{\sqrt{2}} e^{i\theta_{\mathrm{R}}} = \alpha_{\mathrm{R}}(1 + e^{i\theta_{\mathrm{R}}}), \end{cases} \tag{32}$$

which leads to Eq.(27).

Conversely, it is easy to check that Eq. (27) implies the equality $D(H_\gamma) = D(H_\alpha)$. □

*Proof of Theorem 1.* The part (i) just follows from Eqs. (8) and (15).

We employ the same method as in Ref. [27, Theorem 8.26] to prove the part (ii). Note that $D(H_0) \subsetneq D(H_\alpha) \subsetneq D(H_0^*)$ and that $\langle\varphi| - \phi''\rangle = \langle -\varphi''|\phi\rangle + W(\varphi, \phi)$ for all $\varphi, \phi \in D(H_0^*)$ first. Simple calculations lead to the fact that $W(\varphi, \phi) = 0$ for all $\varphi, \phi \in D(H_\alpha)$ given by one of (a) – (d). Thus, $H_\alpha$ is symmetric, i.e., $H_\alpha \subset H_\alpha^*$. Let $\varphi \in D(H_\alpha^*)$. Then, $\langle H_\alpha^*\varphi|\phi\rangle = \langle\varphi|H_\alpha\phi\rangle$ for every $\phi \in D(H_\alpha)$. Thus, $\langle -\varphi''|\phi\rangle = \langle\varphi| -\phi''\rangle$ by Proposition 1 since $H_\alpha \subset H_\alpha^* \subset H_0^*$. It means that $W(\varphi, \phi) = 0$. Take any function $\phi \in D(H_\alpha)$ with $\phi(-\Lambda) \neq 0$ and $\phi(\Lambda) = 0$. Then, using $\phi$ with the boundary condition in the domain (a) we have $\varphi'(-\Lambda) = \alpha_{\mathrm{L}}\varphi(-\Lambda)$. Similarly, using a function $\phi \in D(H_\alpha)$ with $\phi(\Lambda) \neq 0$ and $\phi(-\Lambda) = 0$ we reach the fact that $\varphi'(\Lambda) = \alpha_{\mathrm{R}}\varphi(\Lambda)$. Thus, $\varphi \in D(H_\alpha)$, that is, $H_\alpha^* \subset H_\alpha$. Therefore, $H_\alpha$ is self-adjoint. Since we can similarly handle the other cases, we complete the proof of the part (ii).

The part (iii) for the case ((ii)a) directly follows from Lemma 1. For $\alpha \in \mathbb{R} \times \{\infty\}$ in the case ((ii)b), we expand Eq. (27) to the case $\alpha_{\mathrm{R}} = \infty$ and $\theta_{\mathrm{R}} = \pi$ as $0\infty = 0\alpha_{\mathrm{R}} = 0$. For $\alpha \in \{\infty\} \times \mathbb{R}$ in the case ((ii)c) and $\alpha = (\infty, \infty)$ in the case ((ii)d), we expand Eq. (27) in the same way as in the case ((ii)b). These arguments complete the part (iii). □

**Proposition 2.** *For every vector $\alpha = (\alpha_{\mathrm{L}}, \alpha_{\mathrm{R}}) \in (\mathbb{R} \cup \{\infty\}) \times (\mathbb{R} \cup \{\infty\})$, there is no vector $\gamma = (\gamma_\rightarrow, \gamma_\leftarrow)$ given in Eq. (16) so that $D(H_\alpha) = D(H_\gamma)$. Conversely, for every vector $\gamma = (\gamma_\rightarrow, \gamma_\leftarrow)$ given in Eq. (16), there is no vector $\alpha = (\alpha_{\mathrm{L}}, \alpha_{\mathrm{R}}) \in (\mathbb{R} \cup \{\infty\}) \times (\mathbb{R} \cup \{\infty\})$ so that $D(H_\alpha) = D(H_\gamma)$.*

*Proof.* Let a vector $\alpha = (\alpha_{\mathrm{L}}, \alpha_{\mathrm{R}})$ be in $(\mathbb{R} \cup \{\infty\}) \times (\mathbb{R} \cup \{\infty\})$. Suppose for the sake of contradiction that there is a vector $\gamma = (\gamma_\rightarrow, \gamma_\leftarrow)$ given in Eq. (16) so that $D(H_\alpha) = D(H_\gamma)$. Then, simple calculations lead to a contradiction; $e^{-i\pi/4} = \alpha_{\mathrm{L}} = \alpha_{\mathrm{R}} = e^{i\pi/4}$. Therefore, we prove the first part. In the same way, we can prove the last part. □

**Remark 1.** *We assume that the wave function $\psi(x)$ is in $D(H_0^*)$ for every $\Lambda > 0$ so that*

$$\begin{cases} \lim_{\Lambda\to 0}\psi(-\Lambda) = \psi(0-) = \psi(0) = \psi(0+) = \lim_{\Lambda\to 0}\psi(+\Lambda), \\ \lim_{\Lambda\to 0}\psi'(-\Lambda) = \psi'(0-), \\ \lim_{\Lambda\to 0}\psi'(+\Lambda) = \psi'(0+). \end{cases} \tag{33}$$

*Let $\alpha$, $\alpha_{\mathrm{L}}$, and $\alpha_{\mathrm{R}}$ be given as $-\infty < \alpha, \alpha_{\mathrm{R}} \leq +\infty$ and $-\infty < \alpha_{\mathrm{L}} < +\infty$. When $\alpha_{\mathrm{L}}$ and $\alpha_{\mathrm{R}}$ are arbitrarily given, we define $\alpha$ by $\alpha := \alpha_{\mathrm{R}} - \alpha_{\mathrm{L}}$. Conversely, when $\alpha$ is arbitrarily given, we divide $\alpha$ into $\alpha_{\mathrm{L}}$ and $\alpha_{\mathrm{R}}$ as $\alpha = \alpha_{\mathrm{R}} - \alpha_{\mathrm{L}}$. Let us assume that the boundary condition in Theorem 1 holds for all $\Lambda > 0$. Then, our boundary condition in Theorem 1 tends to the boundary condition in Ref. [24, Eq.(3.1.9)] for the point interaction as $\Lambda \to 0$:*

$$\psi'(0+) - \psi'(0-) = \alpha\,\psi(0). \tag{34}$$

Theorem 1 says that there is no phase factor in the boundary condition when every wave function does not tunnel through the junction. It should be noted that all the cases of Eq. (18) are described as in part (i) of Theorem 1 since $\theta_{\mathrm{L}}$ and $\theta_{\mathrm{R}}$ are independent. On the other hand, in the case where some wave functions tunnel through the junction, we find another type of the boundary conditions, and then, we realize that some phase factors are in this type. We will show this in the next subsection.

### *3.2. Tunneling Schrödinger Particle*

In this subsection, we show that the Schrödinger particle tunneling the junction comes up with another type of the boundary conditions (see Definition 2). Following Eq. (8) again, the unitary operator $U : \mathcal{H}_+(H_0) \longrightarrow \mathcal{H}_-(H_0)$ should be given by

$$UL_+ = \gamma_{\rightarrow} R_- \quad \text{and} \quad UR_+ = \gamma_{\leftarrow} L_- \tag{35}$$

for some $\gamma_{\rightarrow}, \gamma_{\leftarrow} \in \mathbb{C}$ with $|\gamma_{\rightarrow}| = 1 = |\gamma_{\leftarrow}|$. Namely, all wave functions $\psi$ of any self-adjoint extension of $H_0$ satisfying Eq. (35) have the following form:

$$\psi = \psi_0 + c_{\mathrm{L}}(L_+ + \gamma_{\rightarrow} R_-) + c_{\mathrm{R}}(R_+ + \gamma_{\leftarrow} L_-), \tag{36}$$

and moreover, the boundary conditions of $\psi(\Lambda)$ and $\psi'(\Lambda)$ are dependent on those of $\psi(-\Lambda)$ and $\psi'(-\Lambda)$. For the wave functions with the form of Eq.(36), we can find a phase factor in some boundary conditions.

We define some mathematical notions:

**Definition 1.** *A vector $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C}$ belongs to the class $\mathcal{A}$ (i.e., $\vec{\alpha} \in \mathcal{A}$) if the vector $\vec{\alpha}$ satisfies*

**($\mathcal{A}$1)** $\alpha_1\alpha_4^* - \alpha_2^*\alpha_3 = 1$;

**($\mathcal{A}$2)** $\alpha_1\alpha_3^*$, $\alpha_2\alpha_4^* \in \mathbb{R}$.

**Definition 2.** *Fix $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C}$. Then, a wave function $\psi \in D(H_0^*)$ satisfies the boundary conditions $BC(\vec{\alpha})$ if the wave function $\psi$ satisfies*

$$\begin{cases} \psi(\Lambda) = \alpha_1\psi(-\Lambda) + \alpha_2\psi'(-\Lambda), \\ \psi'(\Lambda) = \alpha_3\psi(-\Lambda) + \alpha_4\psi'(-\Lambda). \end{cases} \tag{37}$$

We define a function $F : \mathbb{C}^2 \longrightarrow \mathbb{C}$ by

$$F(z_1, z_2) := |z_1|^2 + \sqrt{2}z_1z_2 + |z_2|^2 - 1 \tag{38}$$

for every $(z_1, z_2) \in \mathbb{C}^2$.

**Definition 3.** *A vector $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C}$ is a solution of the system $\mathcal{S}$ if the vector $\vec{\alpha}$ satisfies*

**($\mathcal{S}$1)** $F(\alpha_1, \alpha_2) = 0 = F(\alpha_3, \alpha_4)$;

**($\mathcal{S}$2)** $\alpha_1 + \alpha_2 e^{-i\pi/4} = \left(\alpha_3 + \alpha_4 e^{-i\pi/4}\right) e^{i3\pi/4}$;

**($\mathcal{S}$3)** $\alpha_1 + \alpha_2 e^{i\pi/4} = \left(\alpha_3 + \alpha_4 e^{i\pi/4}\right) e^{-i3\pi/4}$.

**Example 1.** *Fix $\theta$ with $0 \leq \theta < 2\pi$ arbitrarily. Set $\vec{\alpha}$ as $\alpha_1 = 0$, $\alpha_2 = -e^{i\theta}$, $\alpha_3 = e^{i\theta}$, and $\alpha_4 = 0$. Then, the vector $\vec{\alpha}$ belongs to the class $\mathcal{A}$ and it is a solution of the system $\mathcal{S}$.*

This Example 1, together with the following theorem, secures that the boundary condition $BC(\vec{\alpha})$ can include some phase factors:

**Theorem 2.** *(i) Fix a vector $\vec{\alpha} \in \mathcal{A}$ arbitrarily. Define the action of the Hamiltonian $H_{\vec{\alpha}}$ by $H_{\vec{\alpha}} := -d^2/dx^2$ with*

$$D(H_{\vec{\alpha}}) := \{\psi \in D(H_0^*) \,|\, \psi \text{ satisfies the boundary condition } BC(\vec{\alpha})\}. \tag{39}$$

*Then, $H_{\vec{\alpha}}$ is a self-adjoint extension of $H_0$.*

*(ii) Assume the vector $\vec{\alpha}$ belongs to the class $\mathcal{A}$ and it is a solution of the system $\mathcal{S}$. Define the action of the Hamiltonian $H_\gamma$ by $H_\gamma := -d^2/dx^2$ with $\gamma := (\gamma_\rightarrow, \gamma_\leftarrow)$, and give its domain $D(H_\gamma)$ by the set of all wave functions $\psi$ satisfying Eq.(18):*

$$D(H_\gamma) := \{\psi_0 + c_{\mathrm{L}} f + c_{\mathrm{R}} g \;|\; \psi_0 \in D(H_0), c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}\}. \tag{40}$$

*If $\gamma_{\mathrm{L}}$ and $\gamma_{\mathrm{R}}$ are given by*

$$\gamma_\rightarrow := \left(\alpha_1 + \alpha_2 e^{-i\pi/4}\right) e^{i\sqrt{2}\Lambda} = \left(\alpha_3 + \alpha_4 e^{-i\pi/4}\right) e^{i\left\{\sqrt{2}\Lambda + (3\pi/4)\right\}}, \tag{41}$$

*and*

$$\gamma_\leftarrow := \left(\alpha_1 + \alpha_2 e^{i\pi/4}\right)^{-1} e^{i\sqrt{2}\Lambda} = \left(\alpha_3 + \alpha_4 e^{i\pi/4}\right)^{-1} e^{i\left\{\sqrt{2}\Lambda + (3\pi/4)\right\}}, \tag{42}$$

*then $H_\gamma$ is a self-adjoint extension of $H_0$. Moreover, $H_{\vec{\alpha}} = H_\gamma$.*

Before proving Theorem 2 we note the following five lemmas:

**Lemma 2.** *If $\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}$ satisfy*

$$\alpha_1\alpha_4^* - \alpha_2^*\alpha_3 = 1, \tag{43}$$

$$\alpha_1\alpha_3^*, \;\; \alpha_2\alpha_4^* \in \mathbb{R}, \tag{44}$$

*then $\alpha_j\alpha_{j'}^* \in \mathbb{R}$ for each $j, j' = 1, 2, 3, 4$.*

*Proof.* In the case of $j = j'$, the statement of our lemma is trivial. Thus, we suppose that $j \neq j'$. Equation (43) leads to

$$\alpha_3^* = \alpha_3^*(\alpha_1\alpha_4^* - \alpha_2^*\alpha_3) = \alpha_1\alpha_3^*\alpha_4^* - \alpha_2^*|\alpha_3|^2. \tag{45}$$

Due to the condition (44), multiplying $\alpha_2$ by both sides of this equation gives $\alpha_2\alpha_3^* \in \mathbb{R}$. Also this fact and Eq. (43) say that $\alpha_1\alpha_4^* = 1 + \alpha_2^*\alpha_3 \in \mathbb{R}$ at the same time. Similarly, since Eq. (43) leads to $\alpha_2 = \alpha_2(\alpha_1\alpha_4^* - \alpha_2^*\alpha_3) = \alpha_1\alpha_2\alpha_4^* - |\alpha_2|^2\alpha_3$, we have $\alpha_1^*\alpha_2 \in \mathbb{R}$. Using Eq. (45), we reach $\alpha_3^*\alpha_4 = \alpha_1\alpha_3^*|\alpha_4|^2 - \alpha_2^*\alpha_4|\alpha_3|^2 \in \mathbb{R}$ by the condition (44). We can conclude all the results we desire from the facts that we showed above. □

**Lemma 3.** *If $\alpha_1\alpha_2^*$, $\alpha_3\alpha_4^* \in \mathbb{R}$, then*

$$\alpha_1 + \alpha_2 e^{i\pi/4} \neq 0 \quad \textit{and} \quad \alpha_3 + \alpha_4 e^{i\pi/4} \neq 0. \tag{46}$$

*Proof.* Suppose for the sake of contradiction that (i) $\alpha_1 = -\alpha_2 e^{i\pi/4}$ or (ii) $\alpha_3 = -\alpha_4 e^{i\pi/4}$ holds. In the case where (i) holds, $\mathbb{R} \ni \alpha_1\alpha_2^* = -|\alpha_2|^2 e^{i\pi/4}$, which is a contradiction. In the same way as we did now, we have a contradiction in the case where (ii) holds. □

Straightforward calculations lead to the following two lemmas.

**Lemma 4.** *If $z_1, z_2 \in \mathbb{C}$ satisfy $z_1 z_2^* = \left\{1 - (|z_1|^2 + |z_2|^2)\right\}/\sqrt{2}$, then*

$$\left| z_1 + z_2 e^{\pm i\pi/4} \right| = 1. \tag{47}$$

*Proof.* We have

$$\begin{aligned}\left(z_1 + z_2 e^{\pm i\pi/4}\right)\left(z_1^* + z_2^* e^{\mp i\pi/4}\right) &= |z_1|^2 + |z_2|^2 + z_1 z_2^* \left(\frac{1+i}{\sqrt{2}} + \frac{1-i}{\sqrt{2}}\right) \\ &= |z_1|^2 + |z_2|^2 + z_1 z_2^* \sqrt{2} = 1, \end{aligned} \tag{48}$$

noting $z_1 z_2^* \in \mathbb{R}$ and using the assumption. □

**Lemma 5.** *Let $\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}$ be given so that Eq. (43) and the condition (44) hold. If $\varphi, \phi \in D(H_0^*)$ satisfy the boundary condition $BC(\vec{\alpha})$, then $W(\varphi, \phi) = 0$.*

*Proof.* It follows directly from Eq. (43) and the condition (44) that

$$\begin{aligned}&W(\varphi, \phi) = \\ &\quad \varphi(-\Lambda)^*\phi'(-\Lambda)\left(-1 + \alpha_1^*\alpha_4 - \alpha_2\alpha_3^*\right) + \varphi(-\Lambda)^*\phi(-\Lambda)\left(\alpha_1^*\alpha_3 - \alpha_1\alpha_3^*\right) \\ &\quad + \varphi'(-\Lambda)^*\phi(-\Lambda)\left(\alpha_2^*\alpha_3 + 1 - \alpha_1\alpha_4^*\right) + \varphi'(-\Lambda)^*\phi'(-\Lambda)\left(\alpha_2^*\alpha_4 - \alpha_2\alpha_4^*\right) \\ &\quad = 0, \end{aligned} \tag{49}$$

since $\varphi, \phi \in D(H_0^*)$ satisfy the boundary condition $BC(\vec{\alpha})$. □

We state the last of five lemmas:

**Lemma 6.** *Let $\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}$ be given so that Eq.(46) holds. Then, the boundary condition $BC(\vec{\alpha})$ is equivalent to the following conditions:*

$$\begin{cases} \gamma_{\rightarrow} = \left(\alpha_1 + \alpha_2 e^{-i\pi/4}\right) e^{i\sqrt{2}\Lambda} = \left(\alpha_3 + \alpha_4 e^{-i\pi/4}\right) e^{i3\pi/4} e^{i\sqrt{2}\Lambda}, \\ \gamma_{\leftarrow} = \left(\alpha_1 + \alpha_2 e^{i\pi/4}\right)^{-1} e^{i\sqrt{2}\Lambda} = \left(\alpha_3 + \alpha_4 e^{i\pi/4}\right)^{-1} e^{i3\pi/4} e^{i\sqrt{2}\Lambda}. \end{cases} \tag{50}$$

*Proof.* Let $\psi \in D(H_0^*)$ be an arbitrary wave function satisfying the boundary condition $BC(\vec{\alpha})$. Then, we note that taking this $\psi$ is equivalent to giving $\psi$ with arbitrary $c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}$ so that $\psi = \psi_0 + c_{\mathrm{L}}(L_+ + \gamma_{\rightarrow} R_-) + c_{\mathrm{R}}(R_+ + \gamma_{\leftarrow} L_-)$ by Eqs. (35) and (36). Thus, while the wave function $\psi$ is written at $x = \Lambda$ as $\psi(\Lambda) = c_{\mathrm{L}}\gamma_{\rightarrow} R_+(\Lambda)^* + c_{\mathrm{R}} R_+(\Lambda)$ by Eq. (30), we have

$$\begin{aligned}\psi(\Lambda) &= \alpha_1\psi(-\Lambda) + \alpha_2\psi''(-\Lambda)\\ &= c_{\mathrm{L}}\left(\alpha_1 + \alpha_2 e^{-i\pi/4}\right) R_+(\Lambda) + c_{\mathrm{R}}\left(\alpha_1 + \alpha_2 e^{i\pi/4}\right)\gamma_{\leftarrow} R_+(\Lambda)^*. \end{aligned} \tag{51}$$

Since $c_{\mathrm{L}}, c_{\mathrm{R}}$ are arbitrary, we obtain the first equality of $\gamma_{\rightarrow}$ and $\gamma_{\leftarrow}$ in Eq. (50) individually. Employing the same argument we can express $\gamma_{\rightarrow}$ and $\gamma_{\leftarrow}$ by $\alpha_3, \alpha_4$ as in the second equality of Eq. (50) individually.

We can show directly that Eq. (50) lead to the boundary condition $BC(\vec{\alpha})$ with some straightforward calculations. □

*Proof of Theorem 2.* We employ the same method as in Ref. [27, Theorem 8.26] to prove the part (i). Note that, in the same way as noted in the proof of Theorem 1, $D(H_0) \subsetneq D(H_{\vec{\alpha}}) \subsetneq D(H_0^*)$, and moreover, $\langle\varphi| - \phi''\rangle = \langle -\varphi''|\phi\rangle + W(\varphi, \phi)$ for all $\varphi, \phi \in D(H_0^*)$. Let wave functions $\varphi$ and $\phi$ be in $D(H_{\vec{\alpha}})$. Then, there are $\varphi_0, \phi_0 \in D(H_0)$ and $a_{\mathrm{L}}, a_{\mathrm{R}}, b_{\mathrm{L}}, b_{\mathrm{R}} \in \mathbb{C}$ so that the wave functions $\varphi$ and $\phi$ are written as $\varphi = \varphi_0 + a_{\mathrm{L}} f + a_{\mathrm{R}} g$ and $\phi = \phi_0 + b_{\mathrm{L}} f + b_{\mathrm{R}} g$, respectively. Straightforward calculations lead to

$$\begin{aligned}&W(\varphi, \phi) =\\ &a_{\mathrm{L}}^* b_{\mathrm{L}}\left\{-f(-\Lambda)^* f'(-\Lambda) + f(\Lambda)^* f'(\Lambda) + f'(-\Lambda)^* f(-\Lambda) - f'(\Lambda)^* f(\Lambda)\right\}\\ &+ a_{\mathrm{L}}^* b_{\mathrm{R}}\left\{-f(-\Lambda)^* g'(-\Lambda) + f(\Lambda)^* g'(\Lambda) + f'(-\Lambda)^* g(-\Lambda) - f'(\Lambda)^* g(\Lambda)\right\}\\ &+ a_{\mathrm{R}}^* b_{\mathrm{L}}\left\{-g(-\Lambda)^* f'(-\Lambda) + g(\Lambda)^* f'(\Lambda) + g'(-\Lambda)^* f(-\Lambda) - g'(\Lambda)^* f(\Lambda)\right\}\\ &+ a_{\mathrm{R}}^* b_{\mathrm{R}}\left\{-g(-\Lambda)^* g'(-\Lambda) + g(\Lambda)^* g'(\Lambda) + g'(-\Lambda)^* g(-\Lambda) - g'(\Lambda)^* g(\Lambda)\right\}. \end{aligned} \tag{52}$$

Using Eq. (30), we have

$$\begin{cases} f(-\Lambda) = R_+(\Lambda), & f(\Lambda) = \gamma_{\rightarrow} R_+(\Lambda)^*,\\ f'(-\Lambda) = e^{-i\pi/4} R_+(\Lambda), & f'(\Lambda) = \gamma_{\rightarrow} e^{-i3\pi/4} R_+(\Lambda)^*, \end{cases} \tag{53}$$

$$\begin{cases} g(-\Lambda) = \gamma_{\leftarrow} R_+(\Lambda)^*, & g(\Lambda) = R_+(\Lambda),\\ g'(-\Lambda) = \gamma_{\leftarrow} e^{i\pi/4} R_+(\Lambda)^*, & g'(\Lambda) = e^{i3\pi/4} R_+(\Lambda). \end{cases} \tag{54}$$

Inserting these values into $W(\varphi, \phi)$ obtained above, we have

$$\begin{aligned}W(\varphi, \phi) = &\frac{a_{\mathrm{L}}^* b_{\mathrm{L}} R_+(\Lambda)^* R_+(\Lambda)}{\sqrt{2}}\{\, (-1+i) + |\gamma_{\rightarrow}|^2(-1-i)\\ &\qquad + (1+i) + |\gamma_{\rightarrow}|^2(1-i)\,\}\\ &+ \frac{a_{\mathrm{L}}^* b_{\mathrm{R}}}{\sqrt{2}}\{\, R_+(\Lambda)^{*2}\gamma_{\leftarrow}(-1-i) + R_+(\Lambda)^2\gamma_{\rightarrow}^*(-1+i)\\ &\qquad + R_+(\Lambda)^{*2}\gamma_{\leftarrow}(1+i) + R_+(\Lambda)^2\gamma_{\rightarrow}^*(1-i)\,\}\\ &+ \frac{a_{\mathrm{R}}^* b_{\mathrm{L}}}{\sqrt{2}}\{\, R_+(\Lambda)^2\gamma_{\leftarrow}^*(-1+i) + R_+(\Lambda)^{*2}\gamma_{\rightarrow}(-1-i) \end{aligned}$$

$$
\begin{aligned}
&\qquad\qquad + R_+(\Lambda)^2\gamma_{\leftarrow}^*\,(1-i) + R_+(\Lambda)^{*2}\gamma_{\rightarrow}\,(1+i)\ \}\\
&+\frac{a_{\mathrm{R}}^* b_{\mathrm{R}} R_+(\Lambda)R_+(\Lambda)^*}{\sqrt{2}}\{\ |\gamma_{\rightarrow}|^2\,(-1-i) + (-1+i)\\
&\qquad\qquad\qquad + |\gamma_{\rightarrow}|^2\,(1-i) + (1+i)\ \}\\
&= 0.
\end{aligned} \tag{55}
$$

Thus, $H_{\vec{\alpha}}$ is symmetric, i.e., $H_{\vec{\alpha}} \subset H_{\vec{\alpha}}^*$. Let $\varphi \in D(H_{\vec{\alpha}}^*)$. Then, $\langle H_{\vec{\alpha}}^*\varphi|\phi\rangle = \langle\varphi|H_{\vec{\alpha}}\phi\rangle$ for every $\phi \in D(H_{\vec{\alpha}})$. Thus, $\langle -\varphi''|\phi\rangle = \langle\varphi| -\phi''\rangle$ by Proposition 1 since $H_{\vec{\alpha}} \subset H_{\vec{\alpha}}^* \subset H_0^*$. It means that $W(\varphi,\phi) = 0$. Take any function $\phi \in D(H_\alpha)$ with $\phi(-\Lambda) \neq 0$ and $\phi'(-\Lambda) = 0$. Then, using this $\phi$ with the boundary condition $BC(\vec{\alpha})$, we have

$$\alpha_3\varphi(\Lambda)^* - \alpha_1\varphi'(\Lambda) = -\varphi'(-\Lambda)^*. \tag{56}$$

In the same way, take any function $\phi \in D(H_\alpha)$ with $\phi(-\Lambda) = 0$ and $\phi'(-\Lambda) \neq 0$. Then, using this function $\phi$ with the boundary condition $BC(\vec{\alpha})$, we have

$$\alpha_4\varphi(\Lambda)^* - \alpha_2\varphi'(\Lambda) = \varphi(-\Lambda)^*. \tag{57}$$

It follows from Eqs. (56) and (57) that

$$\begin{cases} -\alpha_2^*\alpha_3\varphi(\Lambda)^* + \alpha_1\alpha_2^*\varphi'(\Lambda) = \alpha_2^*\varphi'(-\Lambda)^*, \\ \alpha_1^*\alpha_4\varphi(\Lambda)^* - \alpha_1^*\alpha_2\varphi'(\Lambda) = \alpha_1^*\varphi(-\Lambda)^*. \end{cases} \tag{58}$$

Summing these two equations gives us the equation:

$$
\begin{aligned}
&(\alpha_1^*\alpha_4 - \alpha_2^*\alpha_3)\,\varphi(\Lambda)^* + (\alpha_1\alpha_2^* - \alpha_1^*\alpha_2)\,\varphi'(\Lambda)\\
&\quad = (\alpha_1\varphi(-\Lambda) + \alpha_2\varphi'(-\Lambda))^*\,.
\end{aligned} \tag{59}
$$

Since $\alpha_1\alpha_2^* \in \mathbb{R}$ by Lemma 2, we have

$$\alpha_1\alpha_2^* - \alpha_1^*\alpha_2 = 0. \tag{60}$$

Since $\alpha_1\alpha_4^* \in \mathbb{R}$ by Lemma 2 again, we have $\alpha_1^*\alpha_4 = \alpha_1\alpha_4^*$. It follows from this fact and $(\mathcal{A}1)$ that

$$\alpha_1^*\alpha_4 - \alpha_2^*\alpha_3 = 1. \tag{61}$$

Combining Eqs. (59), (60), and (61), we can conclude that $\varphi(\Lambda) = \alpha_1\varphi(-\Lambda) + \alpha_2\varphi'(-\Lambda)$. In the same way as demonstrated above, we obtain $\varphi'(\Lambda) = \alpha_3\varphi(-\Lambda) + \alpha_4\varphi'(-\Lambda)$. Thus, $\varphi \in D(H_{\vec{\alpha}})$, that is, $H_{\vec{\alpha}}^* \subset H_{\vec{\alpha}}$. Hence it follows from the two arguments that $H_{\vec{\alpha}}$ is self-adjoint, and thus, part (i) is completed.

Part (ii) directly follows from Lemma 6. □

To see the correspondence of our boundary condition and Eq. (2.2) of Ref. [26], we show the following lemma:

**Lemma 7.** *Let $\vec{\alpha}$ be in the class $\mathcal{A}$. If $\alpha_{j'} \neq 0$, then $\alpha_j\alpha_{j'}^{-1} \in \mathbb{R}$ for $j, j' = 1, 2, 3, 4$.*

*Proof. Proof.* Since $\alpha_j\alpha_{j'}^{-1} = \alpha_j\alpha_{j'}^*|\alpha_{j'}|^{-2} \in \mathbb{R}$ by Lemma 2, we obtain the desired result. □

**Remark 2.** *We assume that the wave function $\psi(x)$ is in $D(H_0^*)$ for every $\Lambda > 0$ so that*

$$\begin{cases} \lim_{\Lambda\to 0}\psi(-\Lambda) = \psi(0-), \\ \lim_{\Lambda\to 0}\psi(+\Lambda) = \psi(0+), \\ \lim_{\Lambda\to 0}\psi'(-\Lambda) = \psi'(0-), \\ \lim_{\Lambda\to 0}\psi'(+\Lambda) = \psi'(0+). \end{cases} \tag{62}$$

*Let $\vec{\alpha}$, $a$, $b$, and $c$ be given as $\vec{\alpha} \in \mathcal{A}$, $a, b \in \mathbb{R}$, and $c \in \mathbb{C}$, respectively. When $\vec{\alpha}$ with $\alpha_2 \neq 0$ is given arbitrarily, based on Lemma 7, we set $a, b$, and $c$ as*

$$a := \alpha_4\alpha_2^{-1} \in \mathbb{R}, \quad b := \alpha_1\alpha_2^{-1} \in \mathbb{R}, \quad c := -(\alpha_2^*)^{-1} \in \mathbb{C}. \tag{63}$$

*So, we have $\alpha_3 = -(c^*)^{-1}(|c|^2 - ab)$. Conversely, when $a, b \in \mathbb{R}$, and $c \in \mathbb{C}$ with $c \neq 0$ are given arbitrarily, we set $\vec{\alpha}$ as*

$$\begin{aligned} &\alpha_1 := -(c^*)^{-1}b, &&\alpha_2 := -(c^*)^{-1}, \\ &\alpha_3 := (c^*)^{-1}(|c|^2 - ab), &&\alpha_4 := -(c^*)^{-1}a. \end{aligned} \tag{64}$$

*Let us assume that the boundary condition in Theorem 2 holds for all $\Lambda > 0$. Then, our boundary condition in Theorem 2 tends to the boundary condition Eq.(2.2) of Ref. [26] as $\Lambda \to 0$:*

$$\begin{aligned} &\psi'(0+) = a\psi(0+) + c\psi(0-), \\ &-\psi'(0-) = c^*\psi(0+) + b\psi(0-). \end{aligned} \tag{65}$$

As a special case of Theorem 2, we take $\vec{\alpha}$ given in Example 1. That is, we set $-\alpha_2 = \alpha_3 = e^{i\theta}$ for every $\theta \in [0, 2\pi)$ and $\alpha_1 = 0 = \alpha_4$. For $\alpha := (\alpha_2, \alpha_3)$ we define the action of the Hamiltonian $H_\alpha$ by $H_\alpha := -d^2/dx^2$, and the domain $D(H_\alpha)$ by

$$D(H_\alpha) := \{\psi \in D(H_0^*) \,|\, \psi(\Lambda) = \alpha_2\psi'(-\Lambda) \text{ and } \psi'(\Lambda) = \alpha_3\psi(-\Lambda)\}. \tag{66}$$

Then, Theorem 2 (i) says that $H_\alpha$ is a self-adjoint extension of $H_0$. This comes up with a concrete phase factor in the boundary condition as an example. Let $\gamma_{\rightarrow}$ and $\gamma_{\leftarrow}$ be given by $\gamma_{\rightarrow} := e^{i\{\theta + \sqrt{2}\Lambda + (3\pi/4)\}}$ and $\gamma_{\leftarrow} := e^{i\{-\theta + \sqrt{2}\Lambda + (3\pi/4)\}}$ for arbitrary $\theta$ with $\theta \in [0, 2\pi)$. For $\gamma := (\gamma_{\rightarrow}, \gamma_{\leftarrow})$ we define the action of the Hamiltonian $H_\gamma$ by $H_\gamma := -d^2/dx^2$, and give its domain $D(H_\gamma)$ by the set of all wave functions $\psi$ satisfying Eq. (36):

$$\begin{aligned} D(H_\gamma) := \{\psi_0 + c_{\mathrm{L}}(L_+ + \gamma_{\rightarrow}R_-) + c_{\mathrm{R}}(R_+ + \gamma_{\leftarrow}L_-) \;| \\ \psi_0 \in D(H_0), c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}\}. \end{aligned} \tag{67}$$

Then, Theorem 2 says that $H_\gamma$ is a self-adjoint extension of $H_0$, and that $H_\alpha$ is represented by $H_\gamma$. Moreover, $H_\alpha$ and $H_\gamma$ have the one-to-one correspondence as in the following theorem:

**Theorem 3.** *Let $\theta \in [0, 2\pi)$ and $\alpha_2, \alpha_3 \in \mathbb{C}$ be given arbitrarily. Then, any subspace $D(H_\gamma)$ and any subspace $D(H_\alpha)$ are equal if and only if the correspondence:*

$$\alpha_2 = -e^{i\theta} \quad \text{and} \quad \alpha_3 = e^{i\theta}. \tag{68}$$

*holds.*

*Proof.* Assume $D(H_\gamma) = D(H_\alpha)$. Take an arbitrary vector $\psi \in D(H_\gamma)$. It is equivalent to take the vector $\psi = \psi_0 + c_{\mathrm{L}} L_+ + c_{\mathrm{R}} R_+ + c_{\mathrm{L}} \gamma_{\rightarrow} R_- + c_{\mathrm{R}} \gamma_{\leftarrow} L_-$ for arbitrary $c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}$ and arbitrary $\psi_0 \in D(H_0)$. By the boundary condition, we have

$$\begin{cases} \gamma_{\rightarrow} R_-(\Lambda) - e^{-i\pi/4}\alpha_2 L_+(-\Lambda) = 0, \\ R_+(\Lambda) - e^{i\pi/4}\alpha_2 \gamma_{\leftarrow} L_-(-\Lambda) = 0, \end{cases} \tag{69}$$

and

$$\begin{cases} e^{-i3\pi/4}\gamma_{\rightarrow} R_-(\Lambda) - \alpha_3 L_+(-\Lambda) = 0, \\ e^{i3\pi/4} R_+(\Lambda) - \alpha_3 \gamma_{\leftarrow} L_-(-\Lambda) = 0. \end{cases} \tag{70}$$

Using Eqs. (30), (31), (69), and (70), we obtain

$$\begin{cases} \gamma_{\rightarrow} - e^{-i\pi/4}\alpha_2 e^{i\sqrt{2}\Lambda} = 0, \\ e^{i\sqrt{2}\Lambda} - e^{i\pi/4}\alpha_2 \gamma_{\leftarrow} = 0, \end{cases} \tag{71}$$

and

$$\begin{cases} e^{-i3\pi/4}\gamma_{\rightarrow} - \alpha_3 e^{i\sqrt{2}\Lambda} = 0, \\ e^{i3\pi/4} e^{i\sqrt{2}\Lambda} - \alpha_3 \gamma_{\leftarrow} = 0. \end{cases} \tag{72}$$

Eq. (68) follows from these four equations.

Conversely, as a corollary of Theorem 2 (ii), Eq. (68) implies the equality $D(H_\gamma) = D(H_\alpha)$. □

For $\gamma_{\rightarrow}$ and $\gamma_{\leftarrow}$ determined by $\alpha_2 = -e^{i\theta}$ and $\alpha_3 = e^{i\theta}$ of Theorem 3, we define two functions $f$ and $g$ by

$$f := L_+ + \gamma_{\rightarrow} R_- \quad \text{and} \quad g := R_+ + \gamma_{\leftarrow} L_-, \tag{73}$$

respectively. We introduce a new inner product $(\ |\ )$ by $(\varphi|\phi) := \langle \varphi|\phi\rangle + \langle \varphi''|\phi''\rangle$. We say that $\varphi$ and $\phi$ are $H_0$-*diagonal* if $(\varphi|\phi) = 0$. Then, we obtain the following:

**Proposition 3.** *Fix an arbitrary $\theta$ with $0 \le \theta < 2\pi$. Define $\gamma_{\rightarrow}$ and $\gamma_{\leftarrow}$ by $\gamma_{\rightarrow} := e^{i\left\{\theta + \sqrt{2}\Lambda + (3\pi/4)\right\}}$ and $\gamma_{\leftarrow} := e^{i\left\{-\theta + \sqrt{2}\Lambda + (3\pi/4)\right\}}$. Then, the following (i) – (iii) hold:*

*(i) $f$ and $g$ defined in Eq. (73) are $H_0$-diagonal;*

*(ii) $f(\Lambda) = e^{i\{\theta + (3\pi/4)\}} f(-\Lambda)$ and $g(\Lambda) = e^{i\{\theta - (3\pi/4)\}} g(-\Lambda)$;*

*(iii) for every $\psi \in D(H_\gamma)$*

$$\psi = \psi_0 + c_{\mathrm{L}} f + c_{\mathrm{R}} g, \tag{74}$$

*where $\psi_0 \in D(H_0)$ and $c_{\mathrm{L}}, c_{\mathrm{R}} \in \mathbb{C}$ are uniquely determined by Eq.(36), and moreover, $\psi_0$, $f$, and $g$ are mutually $H_0$-diagonal.*

*Proof.* The condition (i) is an easy application of Lemma on page 138 of Ref. [22]. Simple calculations lead to the condition (ii). The condition (iii) directly follows from Theorem 3. □

**Remark 3.** *Proposition 3 says that the functions $f$ and $g$ play essential roles to determine wave function $\psi$ around the junction since $\psi_0(x) = 0$ for $x$ in the neighborhood of the junction.*

**Remark 4.** *Proposition 3 (ii) says that the function $f$ (resp. $g$) has the standard Ramsauer-Townsend (RT) effect when $\theta = \pi/4 + 2n\pi$ (resp. $-\pi/4 + 2n\pi$) for each $n \in \mathbb{Z}$. Thus, the functions $f$ and $g$ have a generalization of the RT effect.*

### *3.3. Phase of the tunneling Schrödinger particle and the exact WKB analysis*

In this subsection, we will explain a physical meaning of Proposition 3 using the model of the non-adiabatic transition with the three energy level.

Proposition 3 tells us that the Schrödinger particle leads to the interference by the tunneling effect except for $f = g = 0$ since the wavefunctions $f$ and $g$ get the phase factors $3\pi/4$ and $-3\pi/4$ from the boundary conditions, respectively. As a naive guess, we state the following remark:

**Remark 5.** *By Definition 3 ($\mathcal{S}$1) and ($\mathcal{S}$2), we can rewrite the boundary condition in Proposition 3 (ii) as*

$$f(\Lambda) = -e^{i\{\theta-\pi/4\}} f(-\Lambda) \quad \textit{and} \quad g(\Lambda) = -e^{i\{\theta+\pi/4\}} g(-\Lambda). \tag{75}$$

*We recall that, when we apply the WKB approximation to the Schrödinger particle's barrier-penetration problem, the phase factor $\pi/4$ appears because of the connection formulas (see Ref. [31, Sec. 12]). It should be noted that we have not yet shown whether there is a relation between that phase factor $\pi/4$ and our $\pi/4$ yet.*

We discuss a connection between our phase factors and the WKB analysis in the following. Let us assume the model of the Landau-Zener transition for three levels [29] in the tunneling junction as

$$i\frac{d}{dt}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \eta\left[\begin{pmatrix} b_1t+a & 0 & 0 \\ 0 & b_2t & 0 \\ 0 & 0 & b_3t \end{pmatrix} + \frac{1}{\sqrt{\eta}}\begin{pmatrix} 0 & c_{12} & c_{13} \\ \overline{c_{12}} & 0 & c_{23} \\ \overline{c_{13}} & \overline{c_{23}} & 0 \end{pmatrix}\right]\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}, \tag{76}$$

where $a > 0$ is constant and $b_3 > b_2 > b_1 > 0$. The WKB solution of Eq. (76) is given by Eq. (2.4) of Ref. [29]. The phase factors, which corresponds to one obtained by Proposition 3, appear in a particular model with the connection matrix for the WKB solution, given by by Eq. (2.41) of Ref. [29] from the exact WKB analysis up to the order $\eta^{-1/2}$. The connection matrix is computed through the connection formulas Eqs. (2.27), (2.32), and (2.37) of Ref. [29]. Furthermore, Eq. (76) can be mapped to the BNR equation [30]. According to Ref. [30], the phase factors is obtained by the turning point of the Stokes and anti-Stokes lines. This situation may be experimentally realizable in the systems introduced in Sec. 1.

A keen reader may notice a relationship between the energy crossing and the self-adjointness. However, in this system, the total energy can be preserved while the energy crossing occurs inside the junction. That is, the concept of the self-adjoint

extension effectively may lead to the energy crossing inside the junction remaining the preservation of the total energy. This might be an example of physical meanings on the self-adjointness.

## 4. Conclusion and Discussions

We have considered the phase factor of the one-dimensional Schrödinger particle with the junction like the connected carbon nanotubes and shown that this phase factor depends on the situation of the particle, whether the particle goes through the junction or not. Theorem 1 means that the phase factor of the non-tunneling Schrödinger particle does not appear from the boundary condition of the junction. Proposition 3 means that the phase factor of the tunneling Schrödinger particle appears from the boundary condition of the junction. Physically speaking, the wavefunction of tunneling Schrödinger particle shows the interference pattern. This phase factor corresponds to one obtained by the exact WKB analysis in the model of the non-adiabatic transition with the three energy levels inside the tunneling junction.

There remain the following problems. First, the geometry of the tunneling junction can be taken as the Y-junction scheme [32] in the complex plane. The relationship between the Y-junction scheme and our obtained phase factor has not been shown. Second, our considered model may be also analyzed by the duality of the quantum graph [25, 33]. Finally, the extension to the Dirac particle has not yet been done. This situation can be experimentally realized by the helical edge state in the quantum spin Hall system by the application to the quantum point contact technique [34, 35].

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